



Model order reduction based solver for discontinuous Galerkin element approximation of time-domain Maxwell's equations in dispersive media

Kun Li, Ting-Zhu Huang, Liang Li, Stephane Lanteri

► To cite this version:

Kun Li, Ting-Zhu Huang, Liang Li, Stephane Lanteri. Model order reduction based solver for discontinuous Galerkin element approximation of time-domain Maxwell's equations in dispersive media. IMACS2016 - 20th IMACS WORLD CONGRESS, Dec 2016, Xiamen, China. hal-01416919

HAL Id: hal-01416919

<https://inria.hal.science/hal-01416919>

Submitted on 15 Dec 2016

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Model order reduction based solver for discontinuous Galerkin element approximation of time-domain Maxwell's equations in dispersive media

Kun Li¹, Ting-Zhu Huang¹, Liang Li¹ Stéphane Lanteri²

¹School of Mathematical Sciences, UESTC, P.R. China

²INRIA, 2004 Route des Lucioles, BP 93 06902 Sophia Antipolis Cedex, France

20th IMACS WORLD CONGRESS,
10-14 December 2016.

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

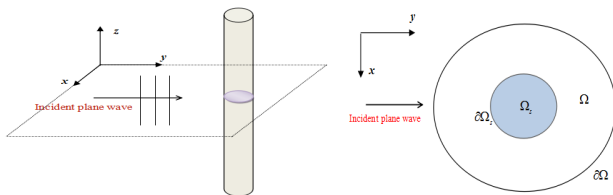
5 Summary

Time-domain Maxwell-Drude equations

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{H}}{\partial t} + \operatorname{curl} \mathbf{E} = 0 \quad \text{in } \Omega \times (0, t_f], \\ \varepsilon_\infty \frac{\partial \mathbf{E}}{\partial t} - \operatorname{curl} \mathbf{H} + \mathbf{J} = 0 \quad \text{in } \Omega \times (0, t_f], \\ \frac{\partial \mathbf{J}}{\partial t} + \gamma_d \mathbf{J} - \omega_d^2 \mathbf{E} = 0 \quad \text{in } \Omega_s \times (0, t_f], \\ \mathbf{E}(\mathbf{x}; 0) = \mathbf{E}_0(\mathbf{x}), \mathbf{H}(\mathbf{x}; 0) = \mathbf{H}_0(\mathbf{x}) \quad \text{in } \Omega, \\ \mathbf{J}(\mathbf{x}; 0) = \mathbf{J}_0(\mathbf{x}) \quad \text{in } \Omega_s. \end{array} \right. \quad (1)$$

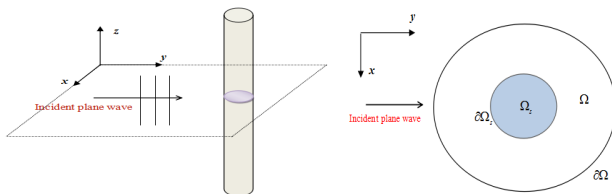
Time-domain Maxwell-Drude equations

$$\begin{cases} \frac{\partial \mathbf{H}}{\partial t} + \operatorname{curl} \mathbf{E} = 0 & \text{in } \Omega \times (0, t_f], \\ \varepsilon_\infty \frac{\partial \mathbf{E}}{\partial t} - \operatorname{curl} \mathbf{H} + \mathbf{J} = 0 & \text{in } \Omega \times (0, t_f], \\ \frac{\partial \mathbf{J}}{\partial t} + \gamma_d \mathbf{J} - \omega_d^2 \mathbf{E} = 0 & \text{in } \Omega_s \times (0, t_f], \\ \mathbf{E}(\mathbf{x}; 0) = \mathbf{E}_0(\mathbf{x}), \mathbf{H}(\mathbf{x}; 0) = \mathbf{H}_0(\mathbf{x}) & \text{in } \Omega, \\ \mathbf{J}(\mathbf{x}; 0) = \mathbf{J}_0(\mathbf{x}) & \text{in } \Omega_s. \end{cases} \quad (1)$$



Time-domain Maxwell-Drude equations

$$\begin{cases} \frac{\partial \mathbf{H}}{\partial t} + \operatorname{curl} \mathbf{E} = 0 & \text{in } \Omega \times (0, t_f], \\ \varepsilon_\infty \frac{\partial \mathbf{E}}{\partial t} - \operatorname{curl} \mathbf{H} + \mathbf{J} = 0 & \text{in } \Omega \times (0, t_f], \\ \frac{\partial \mathbf{J}}{\partial t} + \gamma_d \mathbf{J} - \omega_d^2 \mathbf{E} = 0 & \text{in } \Omega_s \times (0, t_f], \\ \mathbf{E}(\mathbf{x}; 0) = \mathbf{E}_0(\mathbf{x}), \mathbf{H}(\mathbf{x}; 0) = \mathbf{H}_0(\mathbf{x}) & \text{in } \Omega, \\ \mathbf{J}(\mathbf{x}; 0) = \mathbf{J}_0(\mathbf{x}) & \text{in } \Omega_s. \end{cases} \quad (1)$$



- $\Omega \in \mathbb{R}^d$, $d = 2, 3$, t_f is the final physical time.
- \mathbf{E} , \mathbf{H} , and \mathbf{J} respectively denote the electric field, the magnetic field and the dipolar current vector.

Boundary condition

Hard-wall condition [Schmitt N, Scheid C, Lanteri S, et al, JCP, 2016.]:

$$\mathbf{n} \cdot \mathbf{J} = 0 \quad \text{on } \partial\Omega_s. \quad (2)$$

Perfect electric conductor condition (PEC):

$$\mathbf{n} \times \mathbf{E} = 0 \quad \text{on } \Gamma_m. \quad (3)$$

First order Silver-Müller absorbing boundary condition (ABC):

$$\mathbf{n} \times \mathbf{E} + z\mathbf{n} \times (\mathbf{n} \times \mathbf{H}) = \mathbf{n} \times \mathbf{E}^{inc} + z\mathbf{n} \times (\mathbf{n} \times \mathbf{H}^{inc}) \quad \text{on } \Gamma_a. \quad (4)$$

Boundary condition

Hard-wall condition [Schmitt N, Scheid C, Lanteri S, et al, JCP, 2016.]:

$$\mathbf{n} \cdot \mathbf{J} = 0 \quad \text{on } \partial\Omega_s. \quad (2)$$

Perfect electric conductor condition (PEC):

$$\mathbf{n} \times \mathbf{E} = 0 \quad \text{on } \Gamma_m. \quad (3)$$

First order Silver-Müller absorbing boundary condition (ABC):

$$\mathbf{n} \times \mathbf{E} + z \mathbf{n} \times (\mathbf{n} \times \mathbf{H}) = \mathbf{n} \times \mathbf{E}^{inc} + z \mathbf{n} \times (\mathbf{n} \times \mathbf{H}^{inc}) \quad \text{on } \Gamma_a. \quad (4)$$

- $\Gamma_m \cap \Gamma_a = \emptyset$, $\Gamma_m \cup \Gamma_a = \partial\Omega$, \emptyset is an empty set.
- \mathbf{n} denotes the unit normal vector pointing outward to $\partial\Omega$.
- \mathbf{E}^{inc} and \mathbf{H}^{inc} are the incident fields.
- $z = \sqrt{\mu/\varepsilon}$.

Outline

1 Introduction

- Model Problem
- **Motivation**
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

Motivation

At present, most of numerical solvers for (1) with (2)-(4) can be summarized as: FDTD, FETD, FVTD, DGTD, etc. The DGTD methods has many advantages compared with the previous numerical methods:

- the use of unstructured possibly non-conforming meshes.
- easily obtained high order accuracy.
- *hp* -adaptivity.
- natural parallelism.
- ...

Motivation

DOFs of the DGTD method: $N_{dof} = \sum_{i=1}^{n_t} d_i$.

- n_t is the number of elements.
- d_i is the number of DOFs on element i .
 - 1D: $d_i = p + 1$.
 - 2D: $d_i = \frac{1}{2}(p+1)(p+2)$.
 - 3D: $d_i = \frac{1}{6}(p+1)(p+2)(p+3)$.

Motivation

DOFs of the DGTD method: $N_{dof} = \sum_{i=1}^{n_t} d_i$.

- n_t is the number of elements.
- d_i is the number of DOFs on element i .
 - 1D: $d_i = p + 1$.
 - 2D: $d_i = \frac{1}{2}(p+1)(p+2)$.
 - 3D: $d_i = \frac{1}{6}(p+1)(p+2)(p+3)$.

Thus, it becomes an important problem how to get a low dimensional system that has the same response characteristics as the original system, while

- sufficiently accurate numerical solutions.
- far less storage requirements and much lower evaluation time.

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

MOR

- Proper orthogonal decomposition (POD) methods [Holmes P, Lumley J L, Berkooz G, 1998].
- Krylov subspaces methods.
 - Padé-via-Lanczos (PVL) [R Freund, P Feldmann, 1993].
 - the Arnoldi method.
 - the multi-point rational Krylov subspaces [K Gallivan, E Grimme, 1996].
 - ...
- Balanced truncation methods [Moore B, 1981]
- ...

Notations

- K_i : an element of the mesh.
- N_Ω : the set of indices of the mesh elements.
- F_h^I : the union of all interior interfaces.
- F_h^B : the union of all boundary interfaces.
- F_{ij} : the common face of the K_i and K_j , K_j is a adjacent element.
- $\nu_i := \{j | K_i \cap K_j \neq \emptyset\}$: the set of indices of the elements which are neighbors of K_i .

Notations

- K_i : an element of the mesh.
- N_Ω : the set of indices of the mesh elements.
- F_h^I : the union of all interior interfaces.
- F_h^B : the union of all boundary interfaces.
- F_{ij} : the common face of the K_i and K_j , K_j is a adjacent element.
- $\nu_i := \{j | K_i \cap K_j \neq \emptyset\}$: the set of indices of the elements which are neighbors of K_i .

For a face $F_{ij} \in F_h^I$, we define average values $\{\cdot\}$:

$$\{\mathbf{v}\}_{F_{ij}} = \frac{1}{2}(\mathbf{v}_j + \mathbf{v}_i)$$

where \mathbf{v}_j and \mathbf{v}_i respectively stand for the traces of \mathbf{v} on F_{ij} from the interior of K_j and K_i . The finite dimensional subspace can be defined by:

$$\mathbf{V}_h^p := \{\mathbf{v} \in (L^2(\Omega))^3 \mid \mathbf{v}|_{K_i} \in (\mathbb{P}_p(K_i))^3, \forall i \in N_\Omega\}.$$

The restrictions of \mathbf{V}_h^p in Ω_s is denoted by $\tilde{\mathbf{V}}_h^p$.

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

Weak variation

The DG method seeks an approximate solution $(\mathbf{E}_h, \mathbf{H}_h, \mathbf{J}_h)$ in the space $\mathbf{V}_h^p \times \mathbf{V}_h^p \times \tilde{\mathbf{V}}_h^p$ that should satisfy for all K_i in Ω_h :

$$\begin{cases} (\frac{\partial \mathbf{H}_h}{\partial t}, \mathbf{v})_{K_i} + (\text{curl} \mathbf{E}_h, \mathbf{v})_{K_i} = 0, & \forall \mathbf{v} \in \mathbf{V}_h^p, \\ (\varepsilon_\infty \frac{\partial \mathbf{E}_h}{\partial t}, \mathbf{v})_{K_i} - (\text{curl} \mathbf{H}_h, \mathbf{v})_{K_i} + (\mathbf{J}_h, \mathbf{v})_{K_i} = 0, & \forall \mathbf{v} \in \mathbf{V}_h^p, \\ (\frac{\partial \mathbf{J}_h}{\partial t}, \mathbf{v})_{K_i} + (\gamma_d \mathbf{J}_h, \mathbf{v})_{K_i} - (\omega_d^2 \mathbf{E}_h, \mathbf{v})_{K_i} = 0, & \forall \mathbf{v} \in \tilde{\mathbf{V}}_h^p. \end{cases} \quad (5)$$

Using appropriate Green's formulas and replacing the boundary terms by numerical traces \mathbf{E}_h^* and \mathbf{H}_h^* in (5), which are also known as numerical fluxes, we have:

$$\begin{cases} (\frac{\partial \mathbf{H}_h}{\partial t}, \mathbf{v})_{K_i} + (\mathbf{E}_h, \text{curl} \mathbf{v})_{K_i} - \langle \mathbf{E}_h^* \times \mathbf{n}, \mathbf{v} \rangle_{\partial K_i} = 0 & \forall \mathbf{v} \in \mathbf{V}_h^p, \\ (\varepsilon_\infty \frac{\partial \mathbf{E}_h}{\partial t}, \mathbf{v})_{K_i} - (\mathbf{H}_h, \text{curl} \mathbf{v})_{K_i} + (\mathbf{J}_h, \mathbf{v})_{K_i} + \langle \mathbf{H}_h^* \times \mathbf{n}, \mathbf{v} \rangle_{\partial K_i} = 0 & \forall \mathbf{v} \in \mathbf{V}_h^p, \\ (\frac{\partial \mathbf{J}_h}{\partial t}, \mathbf{v})_{K_i} + (\gamma_d \mathbf{J}_h, \mathbf{v})_{K_i} - (\omega_d^2 \mathbf{E}_h, \mathbf{v})_{K_i} = 0 & \forall \mathbf{v} \in \tilde{\mathbf{V}}_h^p. \end{cases}$$

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

Space-discrete formulation

Proper choice of numerical traces \mathbf{E}_h^* and \mathbf{H}_h^* is essential for the correctness and the convergence of the scheme. For the sake of simplicity, we choose to use a fully centered numerical flux, i.e.

$$\mathbf{E}_h^* = \{\mathbf{E}_h\}_{F_{ij}}, \quad \mathbf{H}_h^* = \{\mathbf{H}_h\}_{F_{ij}}, \quad \forall i \in N_\Omega, \quad \forall j \in \nu_i.$$

Replacing surface integrals using centered fluxes in (6) and, re-integrating by parts yields:

$$\begin{cases} \left(\frac{\partial \mathbf{H}_h}{\partial t}, \mathbf{v} \right)_{K_i} = -\frac{1}{2}((\text{curl} \mathbf{v}, \mathbf{E}_h)_{K_i} + (\text{curl} \mathbf{E}_h, \mathbf{v})_{K_i}) + \frac{1}{2} \sum_{l \in \nu_i} \langle \mathbf{E}_l \times \mathbf{n}, \mathbf{v} \rangle_{F_{il}}, \\ \left(\varepsilon_\infty \frac{\partial \mathbf{E}_h}{\partial t}, \mathbf{v} \right)_{K_i} = \frac{1}{2}((\text{curl} \mathbf{v}, \mathbf{H}_h)_{K_i} + (\text{curl} \mathbf{H}_h, \mathbf{v})_{K_i}) - \frac{1}{2} \sum_{l \in \nu_i} \langle \mathbf{H}_l \times \mathbf{n}, \mathbf{v} \rangle_{F_{il}}, \\ \left(\frac{\partial \mathbf{J}_h}{\partial t}, \mathbf{v} \right)_{K_i} = -(\gamma_d \mathbf{J}_h, \mathbf{v})_{K_i} + (\omega_d^2 \mathbf{E}_h, \mathbf{v})_{K_i}. \end{cases} \quad (7)$$

Space-discrete formulation

We now define a set of scalar basis functions φ_{ik} ($1 \leq k \leq d_i$) on the element K_i , and then vectorize the basis functions (as well as the test functions), so in a 3D setting we have $\forall i \in N_\Omega$, $0 \leq k \leq d_i$, the vectorial basis functions

$$\Phi_{ik}^1 = (\varphi_{ik}, 0, 0)^T, \quad \Phi_{ik}^2 = (0, \varphi_{ik}, 0)^T \text{ and } \Phi_{ik}^3 = (0, 0, \varphi_{ik})^T.$$

The test function \mathbf{v} can be chosen as the $3d_i$ vectors Φ_{ik}^m ($1 \leq k \leq d_i$, $1 \leq m \leq 3$). Then the problem (7) can be denoted by an equivalent matrix form:

$$\begin{cases} \mathbb{M}_i \frac{d\mathbf{H}_i}{dt} = -\mathbb{K}_i \mathbf{E}_i + \sum_{l \in \nu_i} \mathbb{S}_{il} \mathbf{E}_l, \\ \varepsilon_\infty \mathbb{M}_i \frac{d\mathbf{E}_i}{dt} = \mathbb{K}_i \mathbf{H}_i - \mathbb{M}_i \mathbf{J}_i - \sum_{l \in \nu_i} \mathbb{S}_{il} \mathbf{H}_l, \\ \frac{d\mathbf{J}_i}{dt} = -\gamma_d \mathbf{J}_i + \omega_d^2 \mathbf{E}_i. \end{cases} \quad (8)$$

Space-discrete formulation

Here, the 3×3 block diagonal mass matrix \mathbb{M}_i , the 3×3 block diagonal stiffness matrix \mathbb{K}_i , and the 3×3 block diagonal surface matrix \mathbb{S}_{il} are defined by their respective diagonal blocks:

$$\begin{cases} (\tilde{\mathbb{M}}_i^m)_{jk} = (\Phi_{ij}^m, \Phi_{ik}^m)_{K_i}, & \text{of size } d_i \times d_i, \quad 1 \leq m \leq 3, \\ (\tilde{\mathbb{K}}_i^m)_{jk} = \frac{1}{2}((\Phi_{ij}^m, \text{curl} \Phi_{ik}^m)_{K_i} + (\text{curl} \Phi_{ij}^m, \Phi_{ik}^m)_{K_i}), & \text{of size } d_i \times d_i, \quad 1 \leq m \leq 3 \\ (\tilde{\mathbb{S}}_{il}^m)_{jk} = \langle \Phi_{ij}^m, \Phi_{lk}^m \times \mathbf{n}_{il} \rangle_{F_{il}}, & \text{of size } d_i \times d_l, \quad l \in \nu_i, \quad 1 \leq m \leq 3, \end{cases}$$

here, d_l denotes the number of DOFs on face $l \in \nu_i$.

Space-discrete formulation

Remark 1. For a metallic boundary face $F_{ij} \in \Gamma_m \cap F_h^B$, the metallic boundary condition is $\mathbf{E}_h|_{F_{ij}} = 0$. We therefore define

$$\mathbf{E}_j|_{F_{ij}} = -\mathbf{E}_i|_{F_{ij}}, \quad \mathbf{H}_j|_{F_{ij}} = \mathbf{H}_i|_{F_{ij}}. \quad (9)$$

For an absorbing boundary face $F_{ij} \in \Gamma_a \cap F_h^B$, we can define

$$\begin{cases} \mathbf{E}_j|_{F_{ij}} = z_i N_{ij} \mathbf{H}_i|_{F_{ij}} + \mathbf{E}_i|_{F_{ij}}^{inc} - z_i N_{ij} \mathbf{H}_i|_{F_{ij}}^{inc}, \\ \mathbf{H}_j|_{F_{ij}} = -z_i^{-1} N_{ij} \mathbf{E}_i|_{F_{ij}} + \mathbf{H}_i|_{F_{ij}}^{inc} + z_i^{-1} N_{ij} \mathbf{E}_i|_{F_{ij}}^{inc}, \end{cases} \quad (10)$$

where $N_{ij} = \begin{pmatrix} 0 & n_{ijz} & -n_{ijy} \\ -n_{ijz} & 0 & n_{ijx} \\ n_{ijy} & -n_{ijx} & 0 \end{pmatrix}$, and $\mathbf{E}_i|_{F_{ij}}^{inc}$, $\mathbf{H}_i|_{F_{ij}}^{inc}$ are given incident fields.

Space-discrete formulation

For all element, we can get a descriptor system of first order in time for (8) as following:

$$\begin{cases} M \frac{d\mathbf{H}_h}{dt} = -\mathbf{K}\mathbf{E}_h + \mathbf{S}^i\mathbf{E}_h + \mathbf{S}^e\mathbf{E}_h + \mathbf{B}^h u_h(t), \\ \varepsilon_\infty M \frac{d\mathbf{E}_h}{dt} = \mathbf{K}\mathbf{H}_h - \mathbf{S}^i\mathbf{H}_h - \mathbf{S}^h\mathbf{H}_h - \mathbf{M}\mathbf{J}_h + \mathbf{B}^e u_e(t), \\ \frac{d\mathbf{J}_h}{dt} = -\gamma_d \mathbf{J}_h + \omega_d^2 \mathbf{E}_h. \end{cases} \quad (11)$$

The descriptor system of first order in time can then be written as:

$$\begin{cases} M\dot{x}(t) = Kx(t) + bu(t), \\ y(t) = p^T x(t), \end{cases} \quad (12)$$

with initial condition $x(0) = x_0 = [\mathbf{E}_0(x), \mathbf{H}_0(x), \mathbf{J}_0(x)]^T$, where $M, K \in R^{N \times N}$, $p, b \in R^N$, and $N = 9N_{dof}$.

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

■ POD-DGTD formulations

- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

POD-DGTD formulations

Let

$$W = [x(t_{n_1}), x(t_{n_2}), \dots, x(t_{n_\ell})] \in R^{N \times \ell}$$

be a collection of **snapshots** of the solution of (12). We compute the singular value decomposition and truncate depending on how fast the singular values decay:

$$W = U \Sigma V^T \approx U_n \Sigma_n V_n^T, \quad n \leq r \leq \ell \ll N.$$

Here, $r = \text{rank}(W)$, U and V are $N \times N$ and $\ell \times \ell$ unitary matrices. Let $U = (\psi_1, \psi_2, \dots, \psi_N)$ and $V = (\phi_1, \phi_2, \dots, \phi_\ell)$, then the POD reduced basis is the set $U_n = \{\psi_i\}_{i=1}^n (n \leq r)$.

POD-DGTD formulations

Then considering the approximation of the state vector $x(t)$ by another state vector, constrained to stay in the subspace spanned by the columns of U_n , namely,

$$x(t) \approx U_n z(t), \quad z(t) \in R^n,$$

yields an linear system with respect to the state variable $z(t)$:

$$\begin{cases} MU_n \dot{z}(t) = KU_n z(t) + bu(t), \\ \tilde{y}(t) = p^T U_n z(t). \end{cases}$$

After left-multiplying the first equation by U_n^T , we have

$$\begin{cases} U_n^T MU_n \dot{z}(t) = U_n^T KU_n z(t) + U_n^T bu(t), \\ \tilde{y}(t) = p^T U_n z(t). \end{cases}$$

Then an n th reduced-order model of the linear system (12) in the time domain is naturally defined, and the quadruples (M_n, K_n, b_n, p_n^T) can be simply expressed as $(U_n^T MU_n, U_n^T KU_n, U_n^T b, p^T U_n)$.

POD-DGTD formulations

Remark 2. For the discrete scheme (8), the number of DOFs ($9N_{dof}$) is very large, but the number DOFs n of the POD-DGTD formulations (22) is very small as we will show from the numerical results.

Remark 3. The choice of the dimension d of the POD basis is not obvious. We denote by $\varepsilon(\psi_1, \psi_2, \dots, \psi_d) = \sum_{j=d+1}^r \lambda_j$ the POD energy or error in the POD basis. If we want the POD energy to be less than some prescribed tolerance ρ , i.e., that

$$\varepsilon(\psi_1, \psi_2, \dots, \psi_n) \leq \rho,$$

we can choose d to be the minimum of positive integer such that

$$\pi(n) = \frac{\sum_{j=1}^n \lambda_j}{\sum_{j=1}^r \lambda_j} \geq 1 - \rho. \quad (13)$$

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

Krylov-subspace based operator exponential approach

Introducing the system matrix A as

$$A = -M^{-1}K,$$

stable field approximations can be computed as [Zimmerling J, Wei L, Urbach P, et al, JCP, 2016]

$$x(t) = u(t) * 2\eta(t) \operatorname{Re}[\eta(A) \exp(-At) M^{-1}b] \quad \text{for } t > 0,$$

where $\eta(t)$ is the Heaviside unit step function. The central approximation of the Krylov subspace techniques described then reads as

$$\exp(-At) M^{-1}b = V_n \exp(-H_n t) \mathbf{e}_1,$$

\mathbf{e}_1 being a first unit basis vector, n being the dimensional of the reduced order system, and V_n , H_n can be obtained by Arnoldi-process or rational Lanczos-process.

The references for Krylov-subspace based operator exponential approach:

- Zimmerling J, Wei L, Urbach P, et al. A Lanczos model-order reduction technique to efficiently simulate electromagnetic wave propagation in dispersive media. *Journal of Computational Physics*, 2016, 315: 348-362.
- Botchev M A. Krylov subspace exponential time domain solution of Maxwell's equations in photonic crystal modeling. *Journal of computational and applied mathematics*, 2016, 293: 20-34.
- Druskin V, Lieberman C, Zaslavsky M. On adaptive choice of shifts in rational Krylov subspace reduction of evolutionary problems. *SIAM Journal on Scientific Computing*, 2010, 32(5): 2485-2496.
- ...

Padé approximation and moment-matching

Taking a Laplace transform for the descriptor system (12), assuming zero initial conditional, and then we obtain the following frequency domain formulation of (12):

$$\begin{cases} sMX(s) = KX(s) + bU(s), \\ Y(s) = p^T X(s) \end{cases} \quad (14)$$

where $X(s)$, $Y(s)$, and $U(s)$ respectively denotes the Laplace transform of $x(x)$, $y(x)$, and $u(x)$. Eliminating $X(s)$ in (14) leads to a transfer function of the original system (12) as

$$H(s) = \frac{Y(s)}{U(s)} = p^T (sM - K)^{-1} b, \quad (15)$$

where $s \in \mathbb{C}$, and $H(s) \in R_{N-1,N}$ is a scalar rational function.

Padé approximation and moment-matching

The Taylor series expansion of $H(s)$ about $s_i \in \mathbb{C}$ ($i = 1, 2, \dots, l$) is given by

$$H(s) = \sum_{j=0}^{\infty} m_j(s_i)(s - s_i)^j, \quad (16)$$

where $m_j(s_i) = p^T [-(s_i M - K)^{-1} M]^j (s_i M - K)^{-1} b$ are called moments about s_i , l is the number of expansion points. We seek a reduced order system such that the Taylor expansion of the corresponding transfer function at s_i has the form

$$H_n(s) = \sum_{j=0}^{\infty} \hat{m}_j(s_i)(s - s_i)^j, \quad (17)$$

where $\hat{m}_j(s_i)$ are called moments about s_i for a reduced order system.

Padé approximation and moment-matching

The function $H_n(s) \in R_{n-1,n}$ is said to be an n th multi-point Padé approximation of $H(s)$ about the expansion point s_i ($i = 1, 2, \dots, l$) if it matches with the moments of $H(s)$ as far as possible, i.e.

$$m_j(s_i) = \hat{m}_j(s_i), \quad j = 0, 1, 2, \dots, j_i - 1, \quad i = 1, 2, \dots, l,$$

where $j_i > 0$ denotes the number of the moments corresponding at s_i , and $n = \sum_{i=1}^l j_i$. Then,

$$H(s) = H_n(s) + \sum_{j=j_i}^{\infty} (m_j(s_i) - \hat{m}_j(s_i))((s - s_i)^j), \quad (18)$$

where the last summation term denotes the error between the frequency response of the original system and that of the reduced-order system. If $l = 1$, (17) is a standard n th Padé approximant for $H(s)$.

Padé approximation and moment-matching

If the transfer function $H_n(s)$ of the reduced-order system is expressed as a scalar rational function

$$H_n(s) = \frac{P_{n-1}(s)}{Q_n(s)}, \quad (19)$$

where the numerator $P_{n-1}(s)$ and the denominator $Q_n(s)$ are defined respectively

$$\begin{cases} P_{n-1}(s) = \sum_{j=0}^{n-1} a_j (s - s)^j, \\ Q_n(s) = 1 + \sum_{j=1}^n b_j (s - s)^j, \end{cases}$$

and the coefficients $\{a_j\}$ and $\{b_j\}$ are unknown, we can obtain a total of $2n$ linear equations by (18) and (19) by collecting the coefficients of the polynomials. Unfortunately, the coefficient matrix of the linear equations, which is called the Hanker matrix, usually is ill-conditioned.

Padé via Lanczos ($l = 1, s_0$)

For the matrix $B = -(K - s_0 M)^{-1} M$, the vector $r = (K - s_0 M)b$, and a left starting vector p , the n th Krylov subspace $\mathcal{K}_n(B, r)$ is spanned by a sequence of n column vectors:

$$\mathcal{K}_n(B, r) = \text{span}\{r, Br, B^2 r, \dots, B^{n-1} r\}.$$

This is sometimes called the right Krylov subspace. When the matrix B is nonsymmetric, there is a left Krylov subspace generated by B^T and a starting vector p defined by

$$\mathcal{K}_n(B^T, p) = \text{span}\{p, B^T p, (B^T)^2 p, \dots, (B^T)^{n-1} p\}.$$

Note that the first $2n$ moments m_i of $H(s)$ are connected with Krylov subspaces through computing the inner products between the left and right Krylov sequences:

$$m_{2i} = ((B^T)^i p)^T \cdot (B^i b)^T, \quad m_{2i+1} = ((B^T)^i p)^T \cdot (B^{i+1} b)^T,$$

for $i = 1, 2, \dots, n-1$.

- └ Reduced-order DG formulations
- └ Krylov subspace based solver

Padé via Lanczos

The left and right Krylov subspaces contain the desired information of moments, but the vectors $B^i r$ and $(B^T)^i p$ are unsuitable as basis vectors. The remedy is to construct more suitable basis vectors $\{v_1, v_2, \dots, v_n\}$ and $\{w_1, w_2, \dots, w_n\}$ such that they span the same desired Krylov subspaces. It is well-known that the Lanczos process is an elegant way to generate the desired basis vectors.

Lanczos process

Give a matrix B , a right starting vector r and a left starting vector p , the Lanczos process generates the basis vector $\{v_i\}$ and $\{w_i\}$, known as the Lanczos vector. Moreover, these Lanczos vector are constructed to be biorthogonal

$$(w_j)^T v_k = 0, \quad \text{for all } j \neq k.$$

The Lanczos vectors can be generated by two three-term recurrences. These recurrences can be stated compactly in matrix form as follows

$$\begin{cases} BV_n = V_n T_n + \rho_{n+1} v_{n+1} \mathbf{e}_n^T, \\ B^T W_n = \tilde{V}_n T_n + \eta_{n+1} w_{n+1} \mathbf{e}_n^T, \end{cases}$$

where T_n and \tilde{T}_n are the tridiagonal matrices.

Reduced Order Model

In general, the application of model order reduction to (12) yields a reduced order model by using the orthogonal projection $x(t) = V_n z(t)$

$$\begin{cases} M_n \dot{z}(t) = K_n z(t) + b_n u(t), \\ \tilde{y}(t) = p_n^T z(t), \end{cases} \quad (20)$$

where $M_n, K_n \in R^{n \times n}$, and $b_n, p_n \in R^n$ have a significantly smaller dimension $n \ll N$ than the original system (12), and

$$M_n = V_n^T M V_n, \quad K_n = V_n^T K V_n, \quad b_n = V_n^T b, \quad p_n = V_n^T p.$$

Why is the simple choice $l = 1$, $s_1 = s_0$?

- If $l > 1$, $s_i \in \mathbb{C}$ ($i = 1, 2, \dots, l$), e.g, the rational Arnoldi method, the selection of suitable expansion points (also called shifts) is crucial for the quality of the resulting reduced order model.
- If $l = 1$, $s_1 = \textit{infinite}$, e.g, PVL with expansion at infinity is fast while the accuracy of the method is very low.

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

Information about test problems:

- The computational domain: the square $\Omega_{\square} = (x, y) \in [0, l] \times [0, l]$.
- The boundary condition: PEC.
- The Drude parameters: $\varepsilon_{\infty} = 3.7362$, $\omega_d = 1.3871\text{e}7$ GHz, $\gamma_d = 4.41544\text{e}4$ GHz.
- Codes: MATLAB 2013b (Memory: 8Gb).
- Method: DG methods with RK_4 , PVL-DGTD methods.

Table: Convergence results for the dispersive cavity problem.

DGTD- \mathbb{P}_1			DGTD- \mathbb{P}_2			DGTD- \mathbb{P}_3			DGTD- \mathbb{P}_4		
h	L^2 -error	r	L^2 -error	r	L^2 -error	r	L^2 -error	r	L^2 -error	r	L^2 -error
3.678e-08	3.482e-08	-	9.364e-10	-	4.161e-11	-	6.735e-13	-	-	-	-
1.839e-08	1.618e-08	1.106	1.965e-10	2.253	5.140e-12	3.017	4.091e-14	4.042	-	-	-
9.194e-09	7.931e-09	1.028	4.678e-11	2.070	6.448e-13	2.995	2.585e-15	3.984	-	-	-
4.597e-09	3.946e-09	1.007	1.161e-11	2.011	8.099e-14	2.993	1.644e-16	3.975	-	-	-

It can be seen that the convergence order of numerical simulation is to satisfy the theoretical convergence order.

Table: Computational performance of the artificial problem.

Mesh	DGTD			PVL-DGTD		
	N	L^2 -error		n	s_0	L^2 -error
\mathbb{P}_1						
M1	3744	3.482e-08	25	1300 <i>f</i>	3.489e-08	
M2	14976	1.618e-08	25	2100 <i>f</i>	1.618e-08	
M3	59904	7.931e-09	35	3500 <i>f</i>	7.930e-09	
\mathbb{P}_2						
M1	7488	9.364e-10	35	1700 <i>f</i>	9.366e-10	
M2	29952	1.965e-10	35	3700 <i>f</i>	1.964e-10	
M3	119808	4.678e-11	90	12000 <i>f</i>	4.684e-11	
\mathbb{P}_3						
M1	12480	4.161e-11	45	1500 <i>f</i>	4.162e-11	
M2	49920	5.140e-12	75	3100 <i>f</i>	5.799e-12	
M3	199680	6.448e-13	100	15000 <i>f</i>	6.518e-13	
\mathbb{P}_4						
M1	18720	6.735e-13	52	2100 <i>f</i>	6.907e-13	
M2	74880	4.092e-14	90	10000 <i>f</i>	4.292e-14	
M3	299520	2.585e-15	150	20000 <i>f</i>	3.473e-15	

✓ the difference between the error calculated by the DGTD method and that calculated by the PVL-DGTD is small.

✓ while the dimension of the reduced order model is much smaller than that of the original system.

Table: Computational performance of the artificial problem.

Mesh	DGTD			PVL-DGTD			Speed-up
	$\overline{T}_{\text{construction}}(\text{s})$	$\overline{T}_{\text{solution}}(\text{s})$		$\overline{T}_{\text{construction}}(\text{s})$	$\overline{T}_{\text{PVL}}(\text{s})$	$\overline{T}_{\text{solution}}(\text{s})$	
\mathbb{P}_1							
M1	0.566	0.405		0.566	0.148	0.026	57.037%
M2	2.535	3.135		2.535	0.990	0.091	65.518%
M3	14.499	29.041		14.499	9.137	1.550	63.200%
\mathbb{P}_2							
M1	0.601	3.109		0.601	0.613	0.059	78.385%
M2	2.873	28.020		2.873	3.725	0.437	85.146%
M3	22.994	285.670		22.994	58.094	8.376	76.732%
\mathbb{P}_3							
M1	0.638	10.680		0.638	2.623	0.147	74.064%
M2	3.765	115.400		3.765	23.464	2.232	77.733%
M3	52.804	1135.300		52.504	224.765	28.818	77.664%
\mathbb{P}_4							
M1	0.896	36.593		0.896	7.689	0.360	78.004%
M2	7.155	334.265		7.155	92.095	4.832	71.003%
M3	126.198	3148.400		126.198	783.482	74.960	72.734%

✓ It is seen that the PVL-DGTD method saves the required CPU time to yield a uniform accuracy level.

- The point with coordinates: $(4.560\text{e-}8, 6.625\text{e-}7)$;
- Methods: DGTD- \mathbb{P}_2 with M2, PVL-DGTD- \mathbb{P}_2 with M2.

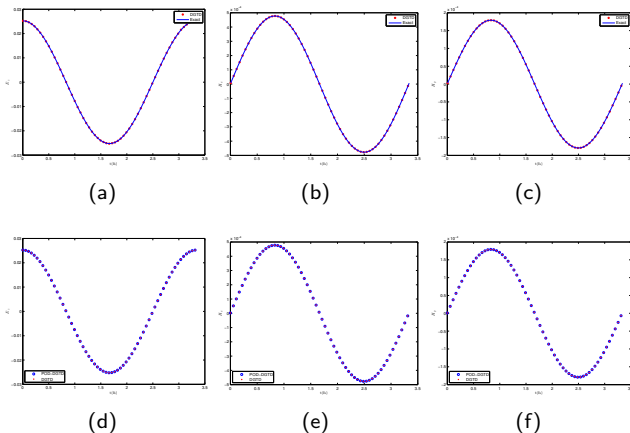


Figure: Comparisons between the usual DGTD methods and the PVL-DGTD methods. (a)~(c): the usual DGTD solutions for E_z , H_x , H_y . (d)~(f): the PVL-DGTD solutions for E_z , H_x , H_y .

■ Time: $t = 1e-6$;

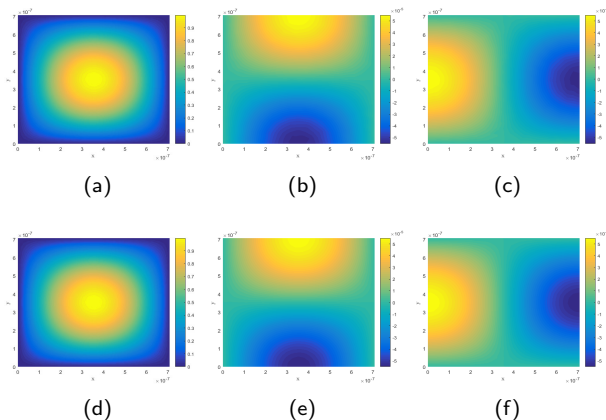


Figure: Comparisons between the usual DGTD methods and the PVL-DGTD methods. (a)~(c): the DGTD solutions for E_z , H_x , H_y . (d)~(f): the PVL-DGTD solutions for E_z , H_x , H_y .

✓ We again find that PVL-DGTD solutions coincide with the DGTD solutions and the analytical solutions.

Outline

1 Introduction

- Model Problem
- Motivation
- Model order reduction

2 DGTD formulations

- Weak variation
- Space-discrete formulation

3 Reduced-order DG formulations

- POD-DGTD formulations
- Krylov subspace based solver
 - Krylov-subspace based operator exponential approach
 - Krylov-subspace based Padé approximation approach

4 Numerical experiments

- Artificial validation case
- Scattering of a plane wave by a Au-nanowire

5 Summary

Information about test problems:

- The computational domain: a gold disk of radius $r = 2nm$.
- The boundary condition: ABC, and propagating along the $-y$ axis.
- The incident plane wave (a sinusoidal modulated Gaussian pulse):

$$\{E_x^{inc}, H_z^{inc}\} \propto \sin(2\pi f_c(t - \tau)) \exp(-(\frac{t - \tau}{\alpha})^2).$$

- The Drude parameters: $\varepsilon_\infty = 1$, $\omega_d = 1.19e4$ THz, $\gamma_d = 141$ THz;
- Codes: MATLAB 2013b (Memory: 8Gb).

Table: Comparisons between the DGTD solutions and the POD-DGTD solutions on CPU times and errors for Au-nanowire.

		Usual DG(a)	Reduced-order DG(b)	Gain	$\max_{n \in [0, N_t]} e_d^n$
MS	\mathbb{P}_p	CPU time(s)	CPU time(s)	CPU_a/CPU_b	
	1	4.253	0.238	17.906	7.431e-12
M1	2	15.637	0.579	27.007	5.028e-12
	1	26.990	1.494	18.070	4.824e-12
M2	2	118.545	5.222	22.703	1.368e-12
	1	866.590	14.744	58.774	8.324e-13
M3	2	3496.236	43.743	79.926	5.531e-13

■ Field distributions. Time: $t = (6 \times 10^{-16})$.

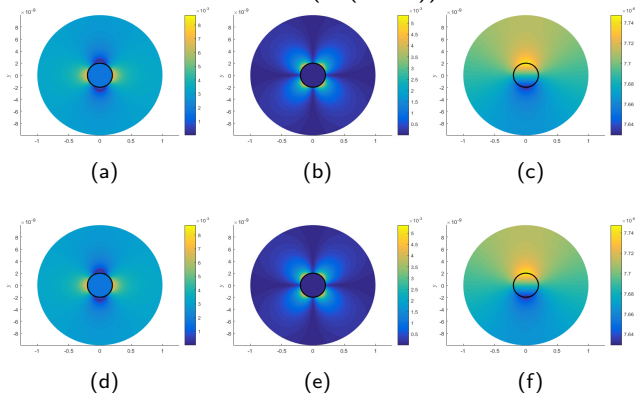


Figure: Field distributions for the simulation of the scattering a plane wave by a gold nanowire. We plot the contour lines of the fields in frequency domain, i.e. the fields are calculated by a DFT from the time-domain solutions by DGTD and POD-DGTD methods. (a)~(c): the DGTD solutions for E_x , E_y , H_z . (d)~(f): the POD-DGTD solutions for E_x , E_y , H_z .

- Field distributions: E_x .
- Time: $t = (6 \times 10^{-16})$.

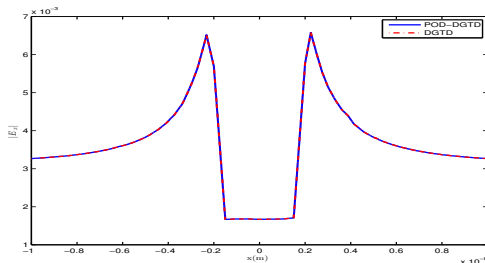


Figure: 1D distribution along the x for the modulus of E_x in the Fourier domain.

Conclusions and Future works

Conclusions:

Conclusions and Future works

Conclusions:

- The reduced-order DG method is developed for saving time;
- The reduced-order DG method has less degrees of freedom compared to the usual DG method;
- Numerical results show their advantages.

Conclusions and Future works

Conclusions:

- The reduced-order DG method is developed for saving time;
- The reduced-order DG method has less degrees of freedom compared to the usual DG method;
- Numerical results show their advantages.

Future works:

Conclusions and Future works

Conclusions:

- The reduced-order DG method is developed for saving time;
- The reduced-order DG method has less degrees of freedom compared to the usual DG method;
- Numerical results show their advantages.

Future works:

- More complex 3d realistic applications should be investigated;
- The error bounds between the usual DG solutions and the reduced-order DG solutions will be derived;
- The extension of this reduce-order method to more general physical model, e.g., Hydrodynamic Drude and generalized non-local modes.
- other MOR methods, such as, rational Krylov subspace technique.

References I



K. Li, T.-Z. Huang, L. Li, L. Stéphane,

A reduced-order discontinuous Galerkin element formulation based on POD method for the time-domain Maxwell's equations in dispersive media.



K. Li, T.-Z. Huang, L. Li, L. Stéphane,

A Krylov subspace based solver for discontinuous Galerkin element approximation of time-domain Maxwell's equations in dispersive media.